

The Kondo Screening Cloud

Ian Affleck*

*Physics Department, Boston University, 590 Commonwealth Ave.
Boston, MA02215*

Renormalization group theory of the Kondo effect predicts that an impurity spin is screened by a conduction electron spread over a large distance of order .1 to 1 micron. This review has the following sections:

1. The Kondo effect and the screening cloud
2. Non-observation of the Kondo cloud in conventional experiments
3. Kondo effect in transmission through a quantum dot
4. Observing the screening cloud in persistent current experiments
5. Side-coupled quantum dot
6. Conclusions

I. THE KONDO EFFECT AND THE SCREENING CLOUD

A single impurity in a metal is described by the Kondo (or s-d) model:

$$H = \sum_{\vec{k}\sigma} \psi_{\vec{k}\sigma}^\dagger \psi_{\vec{k}\sigma} \epsilon_k + J \vec{S}_{\text{imp}} \cdot \vec{S}_{\text{el}}(r=0). \quad (1.1)$$

Here \vec{S}_{imp} is the impurity spin operator (with $S=1/2$) and \vec{S}_{el} is the electron spin density at position \vec{r} . After expanding the electron field, $\psi(\vec{r})$, in spherical harmonics and keeping only the s-wave and linearizing the dispersion relation we obtain a relativistic quantum field theory, defined on a half-line with the impurity at the origin¹. (See fig. I.)



FIG. 1.

The Hamiltonian reduces to:

$$H = iv_F \int_0^\infty dx \left[\psi_L^\dagger \frac{d}{dx} \psi_L - \psi_R^\dagger \frac{d}{dx} \psi_R \right] + 2\pi v_F \lambda \vec{S}_{\text{imp}} \cdot \vec{S}_{\text{el}}(0). \quad (1.2)$$

Here λ is the dimensionless Kondo coupling constant, $J\nu$, where ν is the density of states. To study the problem at low energies, we may apply the renormalization group, integrating out high energy Fourier modes of the electron operators, reducing the band-width, D :

$$d\lambda/d\ln D \approx -\lambda^2 + \dots \quad (1.3)$$

with solution:

$$\lambda_{\text{eff}}(D) \approx \frac{\lambda_0}{1 - \lambda_0 \ln(D_0/D)} + \dots \quad (1.4)$$

The effective coupling becomes $O(1)$ at an energy scale T_K :

$$T_K \approx D e^{-1/\lambda_0}. \quad (1.5)$$

*on leave from Canadian Institute for Advanced Research and Physics Department, University of British Columbia

Here λ_0 is the bare Kondo coupling and D_0 is of order the Fermi energy. After reducing the bandwidth the effective Hamiltonian has a *wave-vector* cut off:

$$|k - k_F| < T_K/v_F \equiv \xi_K. \quad (1.6)$$

This defines a characteristic *length scale* for the Kondo effect; it is typically around .1 to 1 micron.

At low energies, $T \ll T_K$, λ_{eff} seems to get large. This strong coupling physics is easiest to understand in a tight-binding model.

$$H = -t \sum_{j=0}^{\infty} (\psi_j^\dagger \psi_{j+1} + h.c.) + JS_{\text{imp}} \cdot \vec{S}_{\text{el}}(0). \quad (1.7)$$

(See fig. 2.)



FIG. 2.

For $J \gg t$, we simply find the groundstate of the last term in this Hamiltonian. This has 1 electron at site $j = 0$ forming a singlet with the impurity, $|\phi_0\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$. The other electrons are free except that they must not go to $j = 0$ since they would break the singlet. Effectively they feel an infinite repulsion at $j = 0$, corresponding to a $\pi/2$ phase shift. For finite (small) λ_0 , this description only holds at low energies and small $|k - k_F|$. Only long wavelength probes see this simple $\pi/2$ phase shift. This is the basis of Nozières' local Fermi liquid theory of the Kondo effect². The short distance physics is more complicated, involving the singlet formation. Heuristically, we may think of an electron in a wave-function which is spread out over this large distance, ξ_K , which is forming a singlet with the impurity. (More accurately, we should think of the singlet as being formed by a linear superposition of an electron and a hole since there is not necessarily any local modification of the charge density around the impurity.)

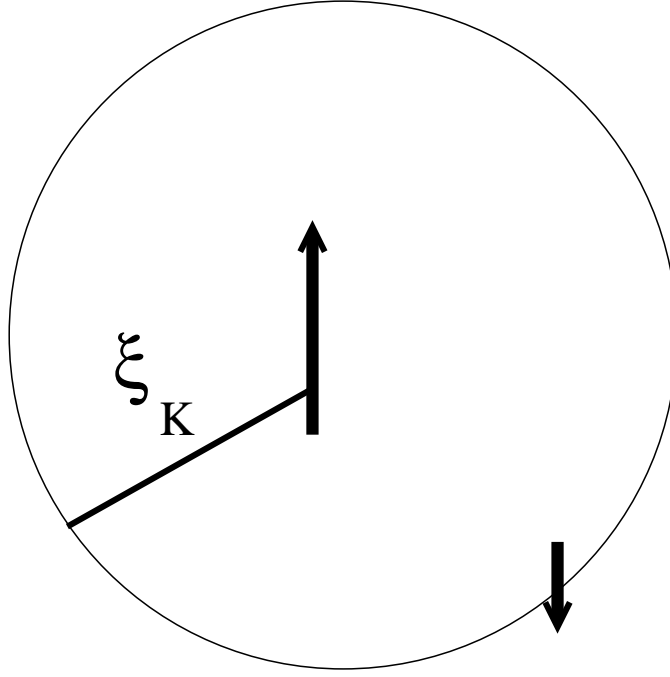


FIG. 3.

II. NON-OBSERVATION OF THE SCREENING CLOUD IN CONVENTIONAL KONDO EXPERIMENTS

This long length scale is surprisingly difficult to observe, perhaps mainly because it is so large.

An important point to realise is that single impurity Kondo behaviour can be observed even when the average inter-impurity separation, R_{imp} , is much greater than ξ_K . This happens because the screening cloud wave-functions from different impurities are nearly orthogonal even when they are strongly overlapping in space³. The condition for single impurity Kondo behavior is probably

$$R_{\text{imp}} \gg \xi_K^{1/3} k_F^{-2/3}. \quad (2.1)$$

This follows from Nozières “exhaustion principle” which states that the number of electrons within $|k - k_F| < \xi_K^{-1}$ should be greater than the number of impurities. This, perhaps optimistic, estimate assumes that if enough states are available the individual screening clouds will manage to be almost orthogonal. However, in a one-dimensional system, the condition is simply that $R_{\text{imp}} \gg \xi_K$.

The Knight shift as a function of distance from an impurity can be measured by nuclear magnetic resonance⁴. At $T = 0$ this takes the form⁵:

$$\chi(r) = \chi_0 + \frac{\cos(2k_F r)}{r^2} f\left(\frac{r}{\xi_K}\right), \quad (2.2)$$

where χ_0 is the susceptibility of the pure system and f is some universal scaling function. The rapid oscillations and the power law pre-factor make this scaling behavior difficult to observe. Typically the signal gets far too small long before r is as large as ξ_K . Furthermore, at such long distances the Knight shift will be given by a superposition of contributions from many impurities.

The charge density around a Kondo impurity varies only over short length scales of $O(1/k_F)$. For instance, in a particle-hole symmetric model, such as a tight-binding model at half-filling, the charge density can easily be proven to be completely uniform. This is connected with “spin-charge separation” in this effectively one-dimensional problem. The Kondo effect takes place purely in the spin sector. Furthermore, the energy and r -dependent density of states, probed by scanning tunnelling microscopy, only varies on short length scales⁶. For the case of a δ -function Kondo interaction, the electron self-energy can be easily shown to have the form:

$$\Sigma(r, \omega) \propto G_0(r, \omega) T(\omega) G_0(r, \omega). \quad (2.3)$$

Here $G_0(r, \omega)$ is the free electron Green’s function, which has trivial dependence on r . $T(\omega)$ has non-trivial dependence on ω and varies on the characteristic energy scale T_K . However, the r -dependence of Σ , and hence the density of states, is trivial.

This stubborn refusal of the Kondo length scale to show up in experiments might make one wonder if it really exists. E. Sørensen and I demonstrated⁷ that it does exist by doing density matrix renormalization group simulations on large finite chains. The system we studied is the one sketched in fig. 2, with an even number of sites L and open boundary conditions and the electron density set at 1/2-filling. In this case the groundstate has spin $S=1/2$. We measured $\langle S_j^z \rangle$ in the groundstate with $S_T^z = +1/2$. This takes the value corresponding to a non-interacting chain with 1 site excised far from the screening cloud ($j \gg \xi_K$). This is $O(1/L)$ and oscillates. At shorter distances $j \leq \xi_K < S_j^z$ exhibits more complicated behavior. We showed that the data appears to collapse onto a single scaling curve when plotted vs. j/ξ_K . (See figs. II and II.) The values of ξ_K obtained from this data collapse had the expected exponential dependence on J .

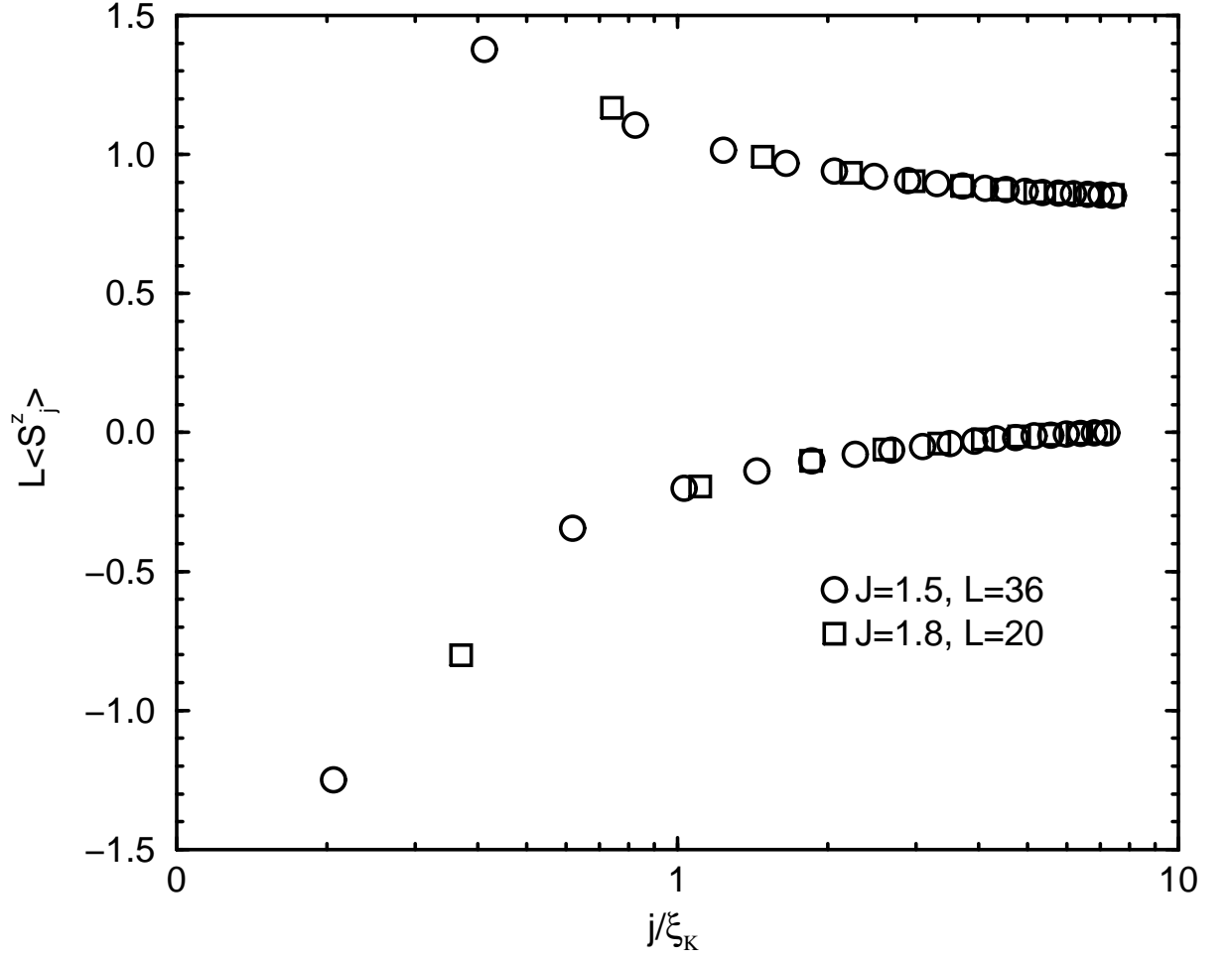


FIG. 4. L times the expectation value of the z-component of the electron spin, $\langle S_j^z \rangle$, as a function of $j/\xi_K(J)$. Two systems are shown: $J = 1.8$, $\xi_K = 2.7$, $L = 20$ and $J = 1.5$, $\xi_K = 4.85$, $L = 36$. Thus in both cases we have $L/\xi_K \approx 7.4$. Clearly the data collapses onto a universal curve.

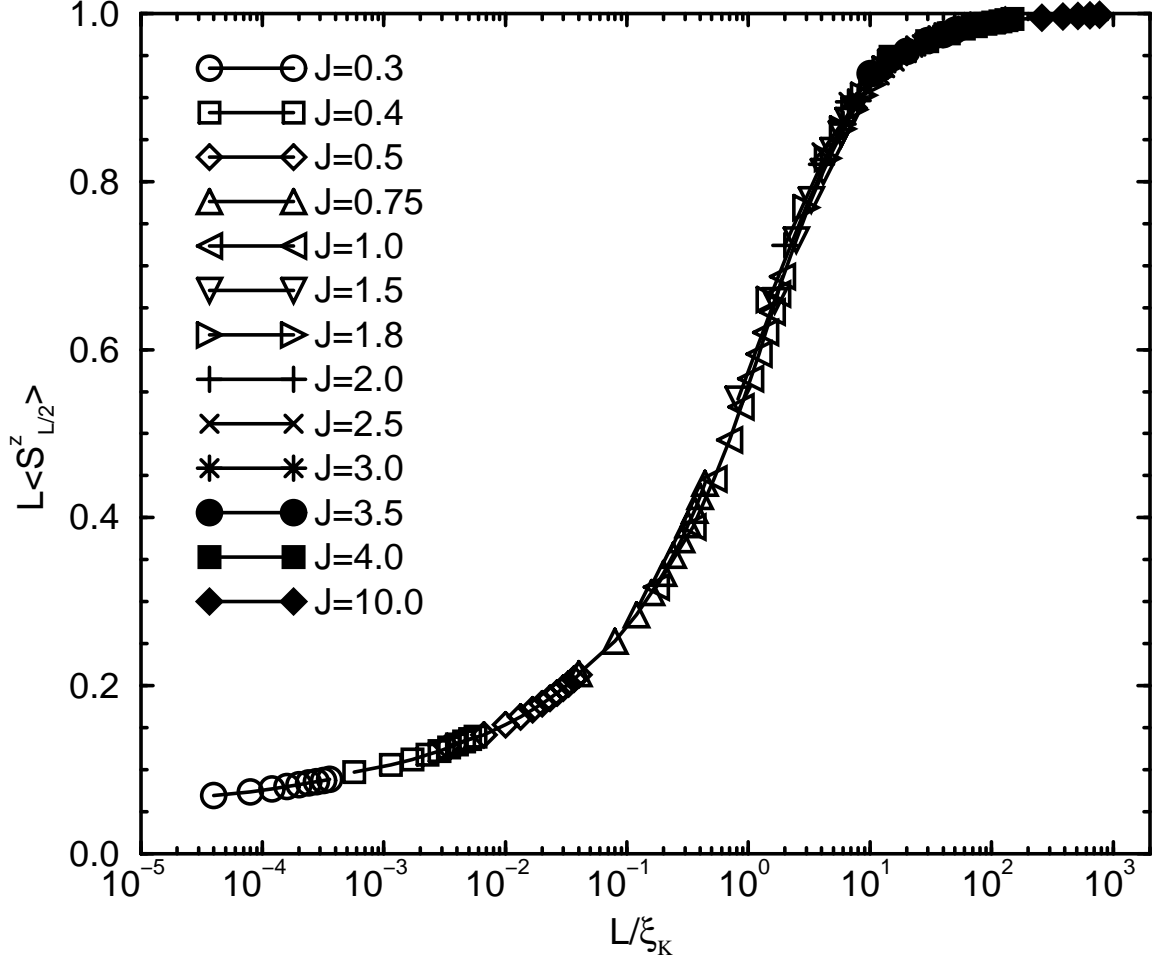


FIG. 5. Logarithmic plot of $L \langle S_{L/2}^z \rangle$ as a function of chain length L/ξ_K for a range of different coupling constants. The initial point corresponds in all cases to $L = 4$. The solid lines are guides to the eye. The strong coupling limit corresponds to $L \langle S_{L/2}^z \rangle \approx 1$

The question remains whether such behaviour could ever be observed experimentally.

III. KONDO EFFECT IN TRANSMISSION THROUGH A QUANTUM DOT

Quantum dots and wires can be made by first forming a two-dimensional electron gas in a semiconductor heterostructure layer and then further confining the electrons by etching and gate voltages varying at the sub-micron scale. Typical dots have been formed with radius around .1 micron containing around 50 electrons. The number of electrons on the dot can be varied in unit steps by varying a gate voltage. Such a system is a single electron transistor. When the tunnelling amplitude between the dots and the leads is weak such a system can exhibit the “Coulomb blockade”. The energy cost to add (or remove) an electron to the dot becomes significant and inhibits conductance through the dot at low T . When the number of electrons on the dot is *odd* it acts like an $S = 1/2$ impurity. Now a type of Kondo effect takes place which corresponds to *perfect transmission* rather than perfect reflection⁸⁻¹⁰. A simplified model which captures the essential physics is the one-dimensional Anderson model^{12,13}. See fig. III.

$$H = -t \left[\sum_{j \leq -2} + \sum_{j \geq 1} \right] (\psi_j^\dagger \psi_{j+1} + h.c.) - t' [\psi_0^\dagger (\psi_{-1} + \psi_1) + h.c.] + \epsilon_0 \psi^\dagger \psi_0 + U n_{0\uparrow} n_{0\downarrow}. \quad (3.1)$$

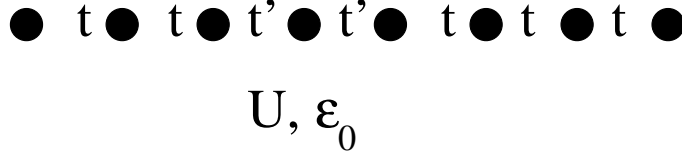


FIG. 6.

The conductance is determined by the transmission amplitude through the dot at the Fermi energy. In the non-interacting case ($U = 0$) there is a transmission resonance when $\epsilon_0 = 2(t'^2 - t^2) \cos k_F$, with a width of $O(t')$. In the Kondo limit, $t' \ll -\epsilon_0, U + \epsilon_0$, the dot acts like an $S=1/2$ impurity with a Kondo interaction:

$$H_{\text{int}} = J(\psi_{-1}^\dagger + \psi_1^\dagger) \frac{\vec{\sigma}}{2} (\psi_{-1} + \psi_1) \cdot \vec{S}_{\text{imp}}. \quad (3.2)$$

Here \vec{S}_{imp} represents the electron spin on the dot and

$$J = 2t'^2 [-1/\epsilon_0 + 1/(U + \epsilon_0)]. \quad (3.3)$$

As usual, we expect J to renormalize to large values as the band-width is reduced. Again it is useful to consider the behaviour for large bare coupling, J . Now the screening electron goes into the symmetric orbital on sites 1 and (-1). Electrons are transmitted through the dot, in this limit, by passing through the anti-symmetric orbital:

$$\psi_a \equiv (\psi_1 - \psi_{-1})/\sqrt{2}. \quad (3.4)$$

The effective low energy Hamiltonian is obtained by taking $J \rightarrow \infty$ and projecting out the symmetric orbital that screens the impurity.

$$H = -t \left[\sum_{j \leq -2} + \sum_{j \geq 1} \right] (\psi_j^\dagger \psi_{j+1} + h.c.) - (t/\sqrt{2}) [-\psi_{-2}^\dagger \psi_a + \psi_a^\dagger \psi_2 + h.c.]. \quad (3.5)$$

This non-interacting Hamiltonian exhibits perfect conductance at half-filling.

In general additional potential scattering terms are induced in the Kondo Hamiltonian of Eq. (3.2) which are also of $O(J)$. This generally occurs unless the Hamiltonian has particle-hole symmetry. (For the Anderson model of Eq. (3.1), exact particle-hole symmetry requires half-filling and $\epsilon_0 = 0$.) If these were added to the large- J effective Hamiltonian they would in general move it off resonance and reduce the conductance. However, another important result about the Kondo model is that such particle-hole symmetry breaking is strictly marginal. These terms do not grow large at low energies but remain of order the bare Kondo coupling. Thus for small bare Kondo coupling the resonance remains pinned at essentially the Fermi energy. Consequently there is a plateau in the transmission as a function of gate voltage, ϵ_0 , over which the conductance is close to the idea value $2e^2/h$, with a width of $O(U)$. Thus, near perfect conductance occurs at low T over the entire range of gate voltage where the occupancy of the dot is an odd integer. Such low temperature conductance plateaux have been observed by the Delft group¹¹.

IV. OBSERVING THE SCREENING CLOUD IN A PERSISTENT CURRENT EXPERIMENT

It is convenient to consider a narrow quantum wire connected to the quantum dot which is eventually connected to macroscopic leads. (See fig. IV.)

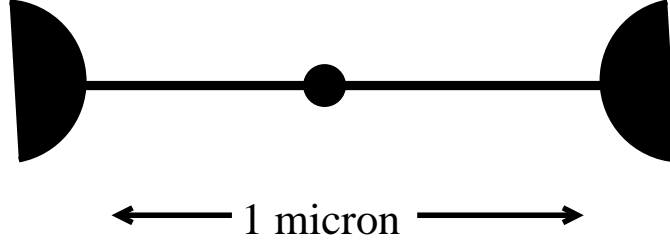


FIG. 7.

Now the screening cloud will live in the leads. It is likely to be considerably larger than the quantum dot and perhaps about equal to the length of the quantum wire leads in some experiments (eg. those of the Delft group). However, these quantum wires are generally connected to macroscopic leads, as sketched in fig. IV. The screening cloud can also exist in the macroscopic section of the leads. Thus it is not obvious how the size of the screening cloud will manifest itself in most experimental set-ups.

One simple possibility (from a theoretical point of view) is to study a closed ring containing a quantum dot. (See fig. IV.)

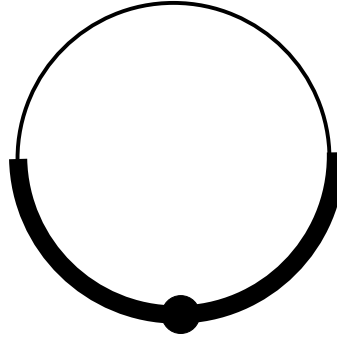


FIG. 8.

Now the screening cloud is trapped on the ring and can't escape into any macroscopic leads. The experimental difficulty is to measure the current through the dot! This could perhaps be done by applying a magnetic field to the ring and measuring the resulting persistent current. When the cloud size, $\xi_K \ll L$, the ring circumference, the perfect transmission through the dot, due to the Kondo effect, implies that the persistent current should be the same as for an ideal ring with no dot. On the other hand, when $\xi_K \gg L$, the Kondo effect doesn't take place; the infrared divergence of the Kondo coupling, λ , is cut off by the finite size of the ring. In this limit the persistent current can be calculated perturbatively in λ .

Analytical expressions for low order perturbation theory can be derived in the tight binding model, for $L \gg 1$, by using continuum limit approximations: linearizing the dispersion relation, etc¹⁴. To include magnetic flux we simply give the hopping terms to the dot phases $\pm\alpha/2$:

$$H_{\text{int}} \rightarrow J(e^{i\alpha/2}\psi_{-1}^\dagger + e^{-i\alpha/2}\psi_1^\dagger)\frac{\vec{\sigma}}{2}(e^{-i\alpha/2}\psi_{-1} + e^{i\alpha/2}\psi_1) \cdot \vec{S}_{\text{imp}}. \quad (4.1)$$

The corresponding flux is $\Phi = (c/2)\alpha$. The persistent current (at $T = 0$) is calculated from the flux-dependence of the groundstate energy:

$$j = -cdE/d\Phi. \quad (4.2)$$

When the total number of electrons (including the electron on the dot), N , is even, there is 1 unpaired electron at the Fermi surface which forms a singlet with the impurity spin. This leads to a contribution of E of first order in λ . When N is odd, E is second order in λ since the groundstate of the $(N - 1)$ non-interacting electrons is a spin singlet. To calculate next order corrections in λ we use the continuum propagator:

$$G(\tau, x) \approx \sum_{n=0}^{\infty} e^{-(v_F \tau + ix)\pi n/L} = 1/(1 - e^{-(v_F \tau + ix)\pi/L}). \quad (4.3)$$

This leads to the following expressions, for N even or odd:

$$\begin{aligned} j_e(\alpha) &\approx \frac{3\pi v_F e}{4L} \{\sin \tilde{\alpha}[\lambda + \lambda^2 \ln Lc] + (1/4 + \ln 2)\lambda^2 \sin 2\tilde{\alpha}\} + \dots \\ j_0(\alpha) &\approx \frac{3\pi v_F e}{16L} \sin 2\alpha[\lambda^2 + 2\lambda^3 \ln Lc'] + \dots \end{aligned} \quad (4.4)$$

Here $\tilde{\alpha}$ is α for $N/2$ even or $\alpha + \pi$ for $N/2$ odd. c and c' are dimensionless constants which we have not bothered to compute. Note that Lj depends on λ and L only through the renormalized coupling constant at scale L :

$$\lambda_{\text{eff}}(L) \approx \lambda + \lambda^2 \ln L + \dots \quad (4.5)$$

This is expected to be exactly true, in all orders of perturbation theory due to standard scaling arguments. Perturbation theory breaks down when $\xi_K \leq L$ but we expect Lj to be given by some universal scaling functions of ξ_K/L . These need to be calculated from large scale numerical simulations, or perhaps using integrability methods. The current in the two limits $L \ll \xi_K$ and $L \gg \xi_K$ are plotted in fig. IV. In the latter case we simply use the result for an ideal ring with no quantum dot. We expect the universal scaling functions to give a smooth cross over between these two limits.

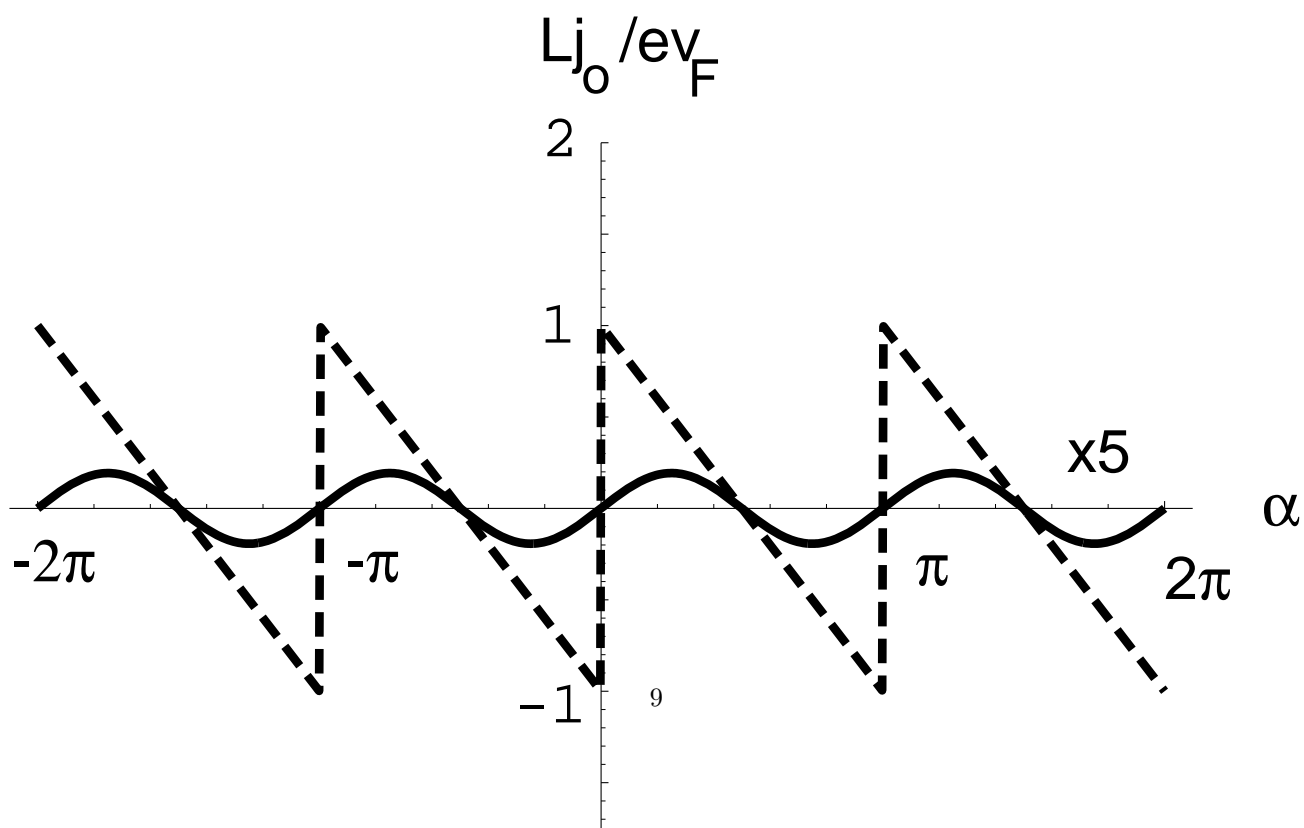
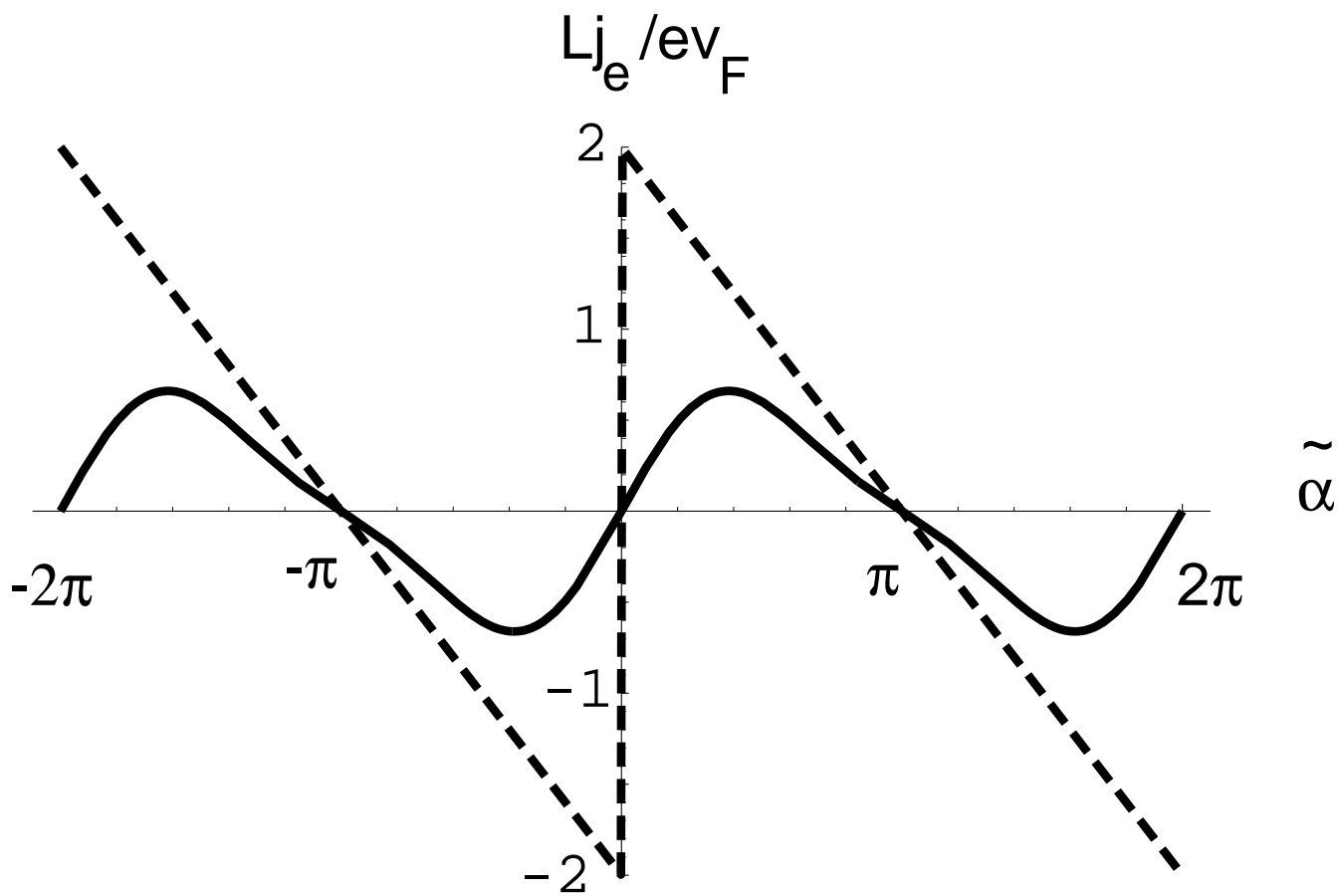


FIG. 9. Persistent current vs. flux for an even or odd number of electrons for $\xi_K/L \approx 50$ (solid line) and for $\xi_K/L \ll 1$ (dashed line). j_o is multiplied $\times 5$ at $\xi_K/L = 50$ for visibility. The solid lines are obtained from Eq. (4.4) using the effective coupling $\lambda(L) \approx 1/\ln(\xi_K/L)$.

Our results disagree with those of several other groups^{16–19}.

There are many effects left out of this simple model which are probably important to a complete understanding of potential experiments in this field. One of these is the presence of several channels in the quantum wire. The Delft experiments suggest about 5 partially filled 1D bands. If we also include more structure in the quantum dot then it might be appropriate to consider a multi-channel Kondo model with all the Kondo couplings, λ_i , different. The corresponding RG equations, to third order, are:²⁰

$$-d\lambda_i/d\ln D = \lambda_i^2 - (1/2)\lambda_i \sum_j \lambda_j^2 + \dots \quad (4.6)$$

For unequal bare couplings, these equations predict that the largest one gets larger and the rest shrink towards zero under renormalization. The physical picture is that one channel screens the quantum dot and has perfect conductance at $T \rightarrow 0$, but the other channels have zero conductance at $T \rightarrow 0$. Thus the basic picture of the Kondo effect is not changed. Assymmetric leads (with different hopping parameters t'_L and t'_R on the two sides of the quantum dot) reduce the conductance and hence the maximum current but we still expect a cross over behaviour at $L \approx \xi_K$. Luttinger liquid interactions in the quantum wire destroys the plateau in the conductance vs. gate voltage, leaving perfect conductance only at one resonant value of the gate voltage²¹ (or none if the interactions are strong enough²²), at least in a one channel model. Non-magnetic disorder in the leads reduces the persistent current even in the limit $L \gg \xi_K$.

V. SIDE-COUPLED DOT

Another interesting model has the quantum dot “side-coupled” to the quantum wire ring, as shown in fig. V. The simplified Anderson Hamiltonian now becomes:

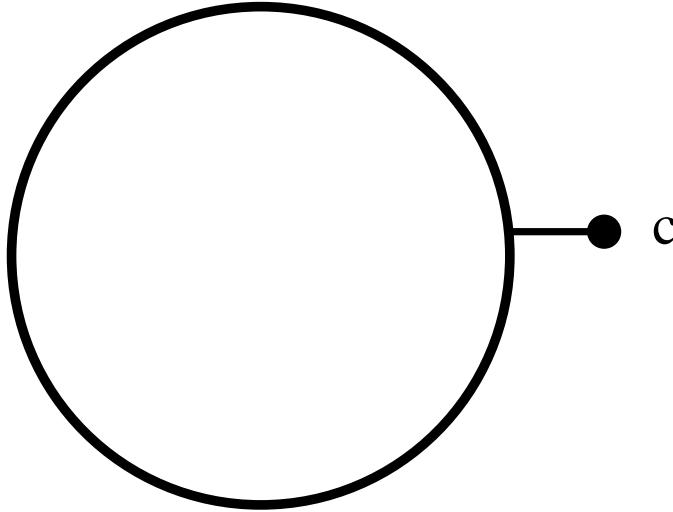


FIG. 10.

$$H = -t \sum_{j=0}^{L-1} [\psi_j^\dagger \psi_{j+1} + h.c.] - t' [\psi_0^\dagger c + h.c.] + \epsilon_0 c^\dagger c + U n_{c\uparrow} n_{c\downarrow}. \quad (5.1)$$

Now when $t' = 0$ there is a perfect current. The growth of the Kondo coupling under renormalization drives the current to 0 for a large ring. The formation of the screening cloud now interferes with the current. Again this is clear in the large J limit. A single electron sits at site 0 and screens the impurity. Other electrons must stay away from 0 corresponding to a $\pi/2$ phase shift in the even

channel. The odd channel wave-functions vanish at 0 so there is no conduction route for electrons in the large J limit. Again we predict scaling behaviour in ξ_K/L . The difference between the two cases may be understood from the formula for the transmission through an impurity with even and odd phase shifts:

$$|T|^2 = \sin^2(\delta_e - \delta_o), \quad (5.2)$$

where δ_e and δ_o are the phase shifts at the Fermi energy in the even and odd channel. When the effective even phase shift goes from near 0 to near $\pi/2$ for a long ring, T can switch between values near 0 and 1. Which occurs in which limit depends on δ_0 .

VI. CONCLUSIONS

The Kondo effect due to spin impurities in metals or due to a quantum dot always involves a large screening cloud whenever the dimensionless Kondo coupling is small. This has never been observed experimentally. In mesoscopic experiments the screening cloud may “escape” into macroscopic leads, in general. This can be avoided in a closed ring experiment where a clear experimental signal emerges from the dependence of the persistent current on the ratio ξ_K/L . How screening manifests itself in transmission experiment with open leads appears much more subtle^{23–25}.

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